

1. INTRODUCTION

This volume of the TRIM.FaTE Technical Support Document (TSD) presents the equations available in the current TRIM.FaTE library that can be used to describe the transport and transformation of chemicals in TRIM.FaTE simulations. These equations are used to simulate the physical, chemical, and biological processes that drive chemical transport and transformation in the environment. As explained in Volume I of this report, the TRIM.FaTE modeling framework can incorporate first-order and higher order equations. At the present time, however, only first-order equations have been included in the TRIM.FaTE library and applied using the model.

First-order transfer between compartments in TRIM.FaTE is described mathematically by **transfer factors**, referred to as T-factors or TFs. This volume documents all of the TF algorithms currently included in the TRIM.FaTE library. A T-factor is the instantaneous flux of the chemical into the receiving compartment normalized by the amount of chemical in the sending compartment (see Section 4.2 in TRIM.FaTE TSD Volume I (U.S. EPA 2002a) for more discussion about T-factors and related issues). That is, $T \times N(t)$ is the instantaneous flux at time t in units of chemical amount/time, where $N(t)$ is the chemical amount in the sending compartment at time t . Thus, the unit for a T-factor is inverse time (in TRIM.FaTE, per day).

Because it is a normalized flux, a large T-factor in itself does not imply that the flux is large; the actual flux also depends on the amount of chemical in the sending compartment. The T-factor is not the same as the fraction of mass transported from the sending to receiving compartment (or transformed or degraded from one chemical form to another) in a given time interval, although the two quantities are related. When the fraction of mass lost is small, these two quantities are approximately the same, but they differ significantly when the fraction of mass lost is larger. In particular, $T = -\ln(1-p)$, where p is the proportion (fraction) of mass lost in one simulation time step, and the units of time are the same as those for T .

The remainder of this volume is organized in seven chapters. Chapter 2 describes the general methods and assumptions used to model fate and transport in TRIM.FaTE, focusing on advection algorithms and the equations to estimate the fraction of the total chemical in a compartment that occurs in each phase (*i.e.*, solid, liquid, vapor) within the compartment. Chapters 3 through 5 present the abiotic transfer factor algorithms for air (Chapter 3), surface water and sediment (Chapter 4), and soil and ground water (Chapter 5). For simplicity, the T-factor algorithms used to describe intermedia transport are presented in only one of the relevant chapters and referenced in the other. Chapters 6 and 7 present the algorithms for transfers between biotic compartment types and between biotic and abiotic compartment types. Chapter 6 describes the algorithms associated with aquatic biota, while Chapter 7 describes those associated with terrestrial biota. Chapters 3 through 7 begin with (or begin each major subsection with) a brief summary of the T-factor algorithms described in the chapter and then explain each algorithm in greater detail. Each chapter also describes supporting equations that are located in the compartment sections of the TRIM.FaTE code library instead of in the T-factor algorithm sections. Chapter 8 provides the references cited in this volume.

This volume includes four appendices. Appendix A presents chemical-specific algorithms for mercury, and Appendix B presents chemical-specific algorithms for polycyclic aromatic hydrocarbons (PAHs). Appendix C describes key aspects of running TRIM.FaTE using the steady-state solution feature. Appendix D lists and describes the input parameters in the current library.

The derivation of T-factors begins in different ways in some chapters, reflecting differences in typical presentations of transfer or partitioning models in the literature among the related disciplines. An effort has been made, however, to use a standard set of variable names throughout this volume (see Acronyms, Abbreviations, and Symbols on pages ix to xii.)